

# OPTIMAL COLLOCATION NODES FOR FRACTIONAL DERIVATIVE OPERATORS

L. FATONE <sup>†</sup> AND D. FUNARO <sup>‡</sup>

**Abstract.** Spectral discretizations of fractional derivative operators are examined, where the approximation basis is related to the set of Jacobi polynomials. The pseudospectral method is implemented by assuming that the grid, used to represent the function to be differentiated, may not be coincident with the collocation grid. The new option opens the way to the analysis of alternative techniques and the search of optimal distributions of collocation nodes, based on the operator to be approximated. Once the initial representation grid has been chosen, indications on how to recover the collocation grid are provided, with the aim of enlarging the dimension of the approximation space. As a results of this process, performances are improved. Applications to fractional type advection-diffusion equations, and comparisons in terms of accuracy and efficiency are made. As shown in the analysis, special choices of the nodes can also suggest tricks to speed up computations.

**Key words.** Fractional derivative, spectral methods, Jacobi polynomials.

**AMS subject classifications.** 65N35, 26A33, 65R10.

**1. Aim of the paper.** Boundary-value problems involving derivatives of fractional order have found increasing interest in the last years. They emerge in a large number of applications, ranging from quantum mechanics to mechanical engineering, chemistry or economics. The literature offers a wide collection of papers. Some references in alphabetical order are for instance: [2], [3], [4], [9], [10], [18], [29], [30], [33], [34], [35], [36], [38], [39], [44]. Analytical solutions via Laplace, Fourier, or Mellin transforms have been proposed in several of the above mentioned papers.

In the framework of numerical approximation, investigations have developed along different paths, including finite-difference methods ([6], [7], [8], [17], [27], [28], [31], [32], [34], [38], [40]) and finite element methods ([5], [9], [10], [48]). More recently, high-order techniques have also been employed. These involve the use of spectral Galerkin methods ([23], [24] [38], [25]) or spectral collocation ([21], [42], [45], [46], [47]). The present paper deals with the last subject.

Using as approximation basis the set of Jacobi polynomials, pseudospectral discretizations of fractional derivative operators are introduced and examined. The idea is to ameliorate the methods recently proposed in [42], [46] and [47]. To this end, a suitable technique is suggested, where the grid used to represent the function to be differentiated, is not necessarily coincident with the collocation grid. This option was studied in [14], [15] and [12] in the framework of standard partial differential equation and in [16] for integral type equations. The scope of using two grids is to enlarge, through a procedure named *superconsistency*, the dimension of the approximation space. The result is an improvement of the overall performance of the method, with very little additional cost.

Asymptotically, i.e. when the number of nodes increases, having different sets for the representation and collocation nodes does not lead to drastic differences. Nevertheless, for lower degree approximating polynomials the gain may be very impressive.

---

<sup>†</sup>Dipartimento di Matematica e Informatica, Università di Camerino, Via Madonna delle Carceri 9, 62032 Camerino (Italy), lorella.fatone@unicam.it, Ph. n.+39-0737-402558, FAX n.+39-0737-632525.

<sup>‡</sup>Dipartimento di Fisica, Informatica e Matematica, Università di Modena e Reggio Emilia, Via Campi 213/B, 41125 Modena (Italy), daniele.funaro@unimore.it, Ph. n.+39-059-2055182, FAX n.+39-059-2055235.

The methodology is then appropriate for stiff problems, where the number of degrees of freedom used for the discretization is still low in order to achieve high accuracy. Examples of this kind are transport-diffusion equations with dominating advective terms. If the polynomial degree is too small to resolve boundary layers, the approximate solution may be very rough. According to [14] and [12], the adoption of a suitable collocation grid leads to excellent improvements. For this reason, in the last section of this paper, we examine a transport-diffusion equation, where the operator contains fractional derivatives. We compare different collocation procedures showing that our approach is actually competitive.

Our discussion also involves a review of the construction of the approximation matrices. In some special cases, we will be able to come out with an explicit expression of the entries of the linear discrete operators. Usually, these quantities are instead computed by introducing further approximation.

Let us note that the concept of *superconsistency* has not to be confused with that of *superconvergence*. In the latter case, the evaluation of the computed solution at special points provides a faster rate of convergence. The idea is borrowed from finite elements and it is a sort of an a posteriori result: from a sequence converging with a certain rate, one can extract a subsequence of point-wise values decaying with improved rate. Some recent superconvergence results in the framework of spectral methods are given for instance in [43], [49]. The aim here is not to improve asymptotically the convergence rate, but to ameliorate the overall performance of existing and spectrally convergent techniques, by working on the possibility of modifying the collocation nodes. Hence, the convergence rate is not going to be higher, however the results, for small values of the discretization parameter, are drastically better in norms defined over the whole interval.

We complete this short introduction with some preliminary definitions. We are concerned with computing fractional derivatives in the interval  $[-1, 1]$ . To this end we work with the Riemann-Liouville fractional operator of order  $\sigma$ :

$$(1.1) \quad (D^\sigma f)(x) = \frac{1}{\Gamma(1-\sigma)} \frac{d}{dx} \int_{-1}^x \frac{f(s)}{(x-s)^\sigma} ds, \quad x > -1.$$

Here  $0 < \sigma < 1$  is the derivative order and  $\Gamma$  denotes the Euler gamma function. Other versions of fractional derivative operators, such as the Caputo's, are available. They are all connected by simple relations, so that, what we are going to develop in the coming sections can be easily extended to other cases. For a general survey of fractional calculus see, for example, [36].

As we said above, our interest is mainly focused on high-order approximation techniques. We will mainly use collocation type methods based on the zeros of Jacobi polynomials. For the reader's convenience, we briefly review some basic and remarkable properties of Jacobi polynomials. First of all, we recall that Jacobi polynomials are denoted by  $P_n^{(\alpha, \beta)}$  where  $n \geq 0$  is the degree and  $\alpha > -1$  and  $\beta > -1$  are given parameters. For  $n \geq 0$ , the  $n$ -th Jacobi polynomial satisfies the following Sturm-Liouville eigenvalue problem in  $[-1, 1]$ :

$$(1.2) \quad (1-x^2) \frac{d^2 P_n^{(\alpha, \beta)}}{dx^2} - ((\alpha + \beta + 2)x + \alpha - \beta) \frac{d P_n^{(\alpha, \beta)}}{dx} + n(n + \alpha + \beta + 1) P_n^{(\alpha, \beta)} = 0.$$

Jacobi polynomials are characterized by the orthogonality relation:

$$(1.3) \quad \int_{-1}^1 P_n^{(\alpha, \beta)}(x) P_k^{(\alpha, \beta)}(x) (1-x)^\alpha (1+x)^\beta dx = 0, \quad \text{if } k \neq n.$$

Moreover, one has for  $n \geq 1$ :

$$(1.4) \quad \int_{-1}^1 \left[ P_n^{(\alpha, \beta)}(x) \right]^2 (1-x)^\alpha (1+x)^\beta dx = \frac{2^{\alpha+\beta+1}}{n! (2n+\alpha+\beta+1)} \frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)}.$$

For  $n \geq 1$ , a very useful relation is:

$$(1.5) \quad \frac{d}{dx} \left[ P_n^{(\alpha, \beta)} \right] = \frac{n+\alpha+\beta+1}{2} P_{n-1}^{(\alpha+1, \beta+1)}.$$

We finally recall that, starting from:

$$(1.6) \quad P_0^{(\alpha, \beta)}(x) = 1, \quad P_1^{(\alpha, \beta)}(x) = \frac{1}{2}(\alpha+\beta+2)x + \frac{1}{2}(\alpha-\beta),$$

higher degree Jacobi polynomials can be determined using the following recurrence relation:

$$(1.7) \quad P_n^{(\alpha, \beta)}(x) = (a_n x + b_n) P_{n-1}^{(\alpha, \beta)}(x) + c_n P_{n-2}^{(\alpha, \beta)}(x), \quad \forall n \geq 2,$$

where:

$$(1.8) \quad a_n = \frac{(2n+\alpha+\beta)(2n+\alpha+\beta-1)}{2n(n+\alpha+\beta)},$$

$$(1.9) \quad b_n = \frac{(\alpha^2 - \beta^2)(2n+\alpha+\beta-1)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)},$$

$$(1.10) \quad c_n = -\frac{(n+\alpha-1)(n+\beta-1)(2n+\alpha+\beta)}{n(n+\alpha+\beta)(2n+\alpha+\beta-2)}, \quad \forall n \geq 2.$$

Ultraspherical polynomials are Jacobi polynomials where  $\alpha = \beta$ . Legendre polynomials are ultraspherical polynomials with  $\alpha = \beta = 0$ . In order to simplify the notation, we set  $P_n = P_n^{(0,0)}$ . Chebyshev polynomials (of the first kind) are related to the ultraspherical polynomials with  $\alpha = \beta = -\frac{1}{2}$ . In fact, they are defined by:

$$(1.11) \quad T_n(x) = \frac{(n! 2^n)^2}{(2n)!} P_n^{(-\frac{1}{2}, -\frac{1}{2})}(x), \quad n \geq 0.$$

For a complete survey of the properties of Jacobi, Legendre and Chebyshev polynomials, as well as other commonly used families of orthogonal polynomials, we refer for instance to [41] and [13].

The most important relation linking Jacobi polynomials with fractional derivatives is represented by the following equation (see [1]):

$$(1.12) \quad \frac{\Gamma(\beta+\mu+1)P_n^{(\alpha-\mu, \beta+\mu)}(-1)}{\Gamma(\beta+1)\Gamma(\mu)P_n^{(\alpha, \beta)}(-1)} \int_{-1}^x \frac{(1+s)^\beta P_n^{(\alpha, \beta)}(s)}{(x-s)^{1-\mu}} ds = (1+x)^{\beta+\mu} P_n^{(\alpha-\mu, \beta+\mu)}(x),$$

$0 < \mu < 1, \quad x \in [-1, 1].$

An interesting version of (1.12) is obtained when  $\alpha = \mu, \beta = -\mu$ . With this choice one has:

$$(1.13) \quad \frac{P_n(-1)}{\Gamma(1-\mu)\Gamma(\mu)P_n^{(\mu, -\mu)}(-1)} \int_{-1}^x \frac{(1+s)^{-\mu} P_n^{(\mu, -\mu)}(s)}{(x-s)^{1-\mu}} ds = P_n(x),$$

where  $0 < \mu < 1$ ,  $x \in [-1, 1]$ . The analysis carried out in this paper is mainly based on the above formula, but it is clear that straightforward generalizations are possible by using the full potentiality of (1.12). We are now ready to study approximations of the operator  $D^\sigma$ ,  $0 < \sigma < 1$ .

**2. A collocation method for  $D^\sigma$ ,  $0 < \sigma < 1$ .** We assume that the nodes  $x_j \in [-1, 1]$ ,  $j = 0, 1, \dots, N$ , are given for some integer  $N \geq 2$ . Their explicit expression will be examined later. From now on we set:  $x_0 = -1$ . Afterwards, we suppose to have a function  $u_N$ , satisfying  $u_N(-1) = 0$  and depending on  $N$  degrees of freedom. Similarly to what has been done in [46] and [47], given  $0 < \mu < 1$ , we suppose that  $u_N$  is expanded in the following Lagrange basis:

$$(2.1) \quad u_N(x) = \sum_{j=1}^N u_N(x_j) H_j(x), \quad 0 < \mu < 1, \quad x \in [-1, 1],$$

where the basis elements  $H_j$ ,  $j = 1, 2, \dots, N$ , are defined as follows:

$$(2.2) \quad H_j(x) = \left( \frac{x_j + 1}{x + 1} \right)^\mu \prod_{\substack{k=0 \\ k \neq j}}^N \left( \frac{x - x_k}{x_j - x_k} \right) = \left( \frac{x + 1}{x_j + 1} \right)^{1-\mu} \prod_{\substack{k=1 \\ k \neq j}}^N \left( \frac{x - x_k}{x_j - x_k} \right),$$

where  $0 < \mu < 1$ ,  $x \in [-1, 1]$ . Indeed, we have the Kronecker delta property  $H_j(x_m) = \delta_{jm}$ ,  $j, m = 1, 2, \dots, N$ . Basically, we have to deal with a polynomial of degree  $N$ , suitably corrected at the point  $x_0 = -1$ . Except for this initial setting, our approach is going to be different from the one followed in [46], [47].

By the linearity of the fractional differential operator  $D^\sigma$ ,  $0 < \sigma < 1$ , we are allowed to write:

$$(2.3) \quad (D^\sigma u_N)(x) = \sum_{j=1}^N u_N(x_j) (D^\sigma H_j)(x), \quad 0 < \sigma < 1, \quad x \in [-1, 1],$$

so that we need to evaluate the effect of applying  $D^\sigma$ ,  $0 < \sigma < 1$ , to each element of the basis  $H_j$ ,  $j = 1, 2, \dots, N$ .

In order to use formula (1.13), we are going to represent the elements  $H_j$ ,  $j = 1, 2, \dots, N$ , in the following equivalent form:

$$(2.4) \quad H_j(x) = (x + 1)^{-\mu} \sum_{n=1}^N c(j, n) \left[ P_n^{(\mu, -\mu)}(x) - P_n^{(\mu, -\mu)}(-1) \right].$$

Note that the right-hand side of (2.4) actually vanishes for  $x_0 = -1$ , because  $H_j(x) \approx (x + 1)^{1-\mu}$  in the neighborhood of that point.

The difficulty is to pass from one representation of  $u_N$  to the other, that is to pass from the representation (2.1) of  $u_N$  with  $H_j$ ,  $j = 1, 2, \dots, N$ , defined in (2.2) to the representation (2.1) of  $u_N$  with  $H_j$ ,  $j = 1, 2, \dots, N$ , defined in (2.4).

Searching for explicit formulas is rather cumbersome and may lead to an expensive and ill-conditioned algorithm, especially if one passes through the monomial basis  $x^k$ ,  $k = 1, 2, \dots, N$  (which is the procedure followed in [42]). The solution we suggest is to solve a simple linear system. In fact, by observing that  $H_j(x_m) = \delta_{jm}$ ,  $j, m = 1, 2, \dots, N$ , one can evaluate equation (2.4) at  $x = x_m$ ,  $m = 1, 2, \dots, N$ , obtaining:

$$(2.5) \quad (x_m + 1)^{-\mu} \sum_{n=1}^N c(j, n) \left[ P_n^{(\mu, -\mu)}(x_m) - P_n^{(\mu, -\mu)}(-1) \right] = \delta_{jm}.$$

TABLE 1  
Condition number of  $A_N$  when  $x_j = -\cos(j\pi/N)$ ,  $j = 1, 2, \dots, N$ , and  $\mu = 0.5$ .

$N$	$\text{cond}(A_N)$
5	3.7240
10	8.9481
20	19.0645
50	50.3533
100	103.4209

By introducing the  $N \times N$  matrix:

$$(2.6) \quad A_N = \{a_{j,n}\} = \left\{ (x_j + 1)^{-\mu} \left[ P_n^{(\mu, -\mu)}(x_j) - P_n^{(\mu, -\mu)}(-1) \right] \right\},$$

where  $j, n = 1, 2, \dots, N$ , we get the expansion coefficients  $c(j, n)$  as the entries of the matrix  $A_N^{-1}$ . This computation is relatively cheap and the condition number of  $A_N$  is quite acceptable, as one can check, for example, by examining Table 1. This test is related to the distribution of nodes:

$$(2.7) \quad x_j = -\cos(j\pi/N), \quad j = 1, 2, \dots, N.$$

The nodes  $x_j$ ,  $j = 1, 2, \dots, N$  defined in (2.7) are the zeros of  $T'_N$  (the derivative of the  $N$ -th Chebyshev polynomial) with the addition of the point  $x_N = 1$ .

Table 1 shows that the growth of the condition number of  $A_N$  is clearly proportional to  $N$  in this case. In some circumstances the evaluation of  $c(j, n)$ ,  $j, n = 1, 2, \dots, N$ , is straightforward, as it will be checked in §5.

We are now ready to compute the fractional derivative of all  $H_j$ ,  $j = 1, 2, \dots, N$ . For this, we require that  $\mu = 1 - \sigma$ . Therefore using (1.13) we obtain:

$$\begin{aligned}
 (D^\sigma H_j)(x) &= (D^{1-\mu} H_j)(x) = \frac{1}{\Gamma(\mu)} \frac{d}{dx} \int_{-1}^x \frac{H_j(s)}{(x-s)^{1-\mu}} ds \\
 (2.8) \quad &= \frac{1}{\Gamma(\mu)} \sum_{n=1}^N c(j, n) \frac{d}{dx} \int_{-1}^x \frac{(1+s)^{-\mu} P_n^{(\mu, -\mu)}(s)}{(x-s)^{1-\mu}} ds \\
 &= \sum_{n=1}^N \frac{\Gamma(1-\mu) P_n^{(\mu, -\mu)}(-1)}{P_n(-1)} c(j, n) P'_n(x) = \sum_{n=1}^N \frac{\Gamma(n-\mu+1)}{n!} c(j, n) P'_n(x).
 \end{aligned}$$

In the last passage we used the following relation (see [41]):

$$(2.9) \quad P_n^{(\alpha, \beta)}(-1) = (-1)^n \binom{n+\beta}{n} = (-1)^n \frac{\Gamma(n+\beta+1)}{n! \Gamma(\beta+1)},$$

where  $\alpha = \mu$  and  $\beta = -\mu$ . In particular, one has  $P_n(-1) = (-1)^n$ . In computing (2.8) we eliminated a term. In truth, that was actually zero. Indeed, by recalling that  $P_0^{(\alpha, \beta)}(x) = 1$ ,  $\forall x$ , we have:

$$\begin{aligned}
 \frac{d}{dx} \int_{-1}^x \frac{(1+s)^{-\mu} P_n^{(\mu, -\mu)}(-1)}{(x-s)^{1-\mu}} ds &= P_n^{(\mu, -\mu)}(-1) \frac{d}{dx} \int_{-1}^x \frac{(1+s)^{-\mu} P_0^{(\mu, -\mu)}(s)}{(x-s)^{1-\mu}} ds \\
 (2.10) \quad &= P_n^{(\mu, -\mu)}(-1) \frac{\Gamma(1-\mu) \Gamma(\mu) P_0^{(\mu, -\mu)}(-1)}{P_0(-1)} P'_0(x) = 0.
 \end{aligned}$$

Finally, given  $0 < \sigma < 1$ , by previously computing the coefficients  $c(j, n)$ , we can assemble the  $N \times N$  fractional derivative matrix  $D_N^\sigma$  by setting:

$$(2.11) \quad D_N^\sigma = \{d_{i,j}^\sigma\} = \sum_{n=1}^N \frac{\Gamma(n - \mu + 1)}{n!} c(j, n) P_n'(z_i), \quad i, j = 1, 2, \dots, N.$$

In (2.11) the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N$ , do not necessarily coincide with the nodes  $x_j$ ,  $j = 1, 2, \dots, N$ .

In the end, for a given  $0 < \sigma < 1$ , let us suppose to have the fractional differential problem:

$$(2.12) \quad D^\sigma u = g, \quad u(-1) = 0,$$

with given right-hand side  $g$ . We then propose to approximate (2.12) by the following discrete problem:

$$(2.13) \quad D_N^\sigma u_N = g_N, \quad u_N(-1) = 0,$$

where  $D_N^\sigma$  replaces  $D^\sigma$ ,  $u_N$  is the discrete solution and  $g_N$  is the interpolant of  $g$  at the collocation nodes.

In the following sections we will specify how to properly choose representation and collocation nodes in order to achieve optimal results.

**3. Higher-order fractional derivative operators.** Fractional derivatives of order greater than one can be obtained by composition. In particular fractional derivatives of order  $1 + \sigma$ ,  $0 < \sigma < 1$ , can be computed as follows:

$$(3.1) \quad D^{1+\sigma} = D D^\sigma,$$

where  $D = D^1$  is the standard first derivative operator. Similarly, one can handle derivatives of the form  $D^{k+\sigma}$ ,  $0 < \sigma < 1$ , where  $k$  is an integer such that  $k \geq 1$ .

Let us note that, given an integer  $k \geq 1$ , standard derivatives  $D^k$  of order  $k$  of the basis functions  $H_j$  in (2.4) are evaluated as follows:

$$(3.2) \quad (D^k H_j)(x) = \sum_{n=1}^N c(j, n) \frac{d^k}{dx^k} \left[ (x+1)^{-\mu} (P_n^{(\mu, -\mu)}(x) - P_n^{(\mu, -\mu)}(-1)) \right], \quad k \geq 1.$$

For example in §6, we will approach a differential equation involving the operator  $-D^2 + K D^\sigma$ , where  $K$  is a given constant. By taking  $k = 2$  in (3.2) and combining (2.8) and (3.2), one gets for  $j = 1, 2, \dots, N$ :

$$(3.3) \quad \begin{aligned} (-D^2 H_j + K D^\sigma H_j)(x) = & \sum_{n=1}^N c(j, n) \left( -\frac{d^2}{dx^2} \left[ (x+1)^{-\mu} P_n^{(\mu, -\mu)}(x) \right] \right. \\ & \left. + \mu(\mu+1)(x+1)^{-\mu-2} P_n^{(\mu, -\mu)}(-1) + K \frac{\Gamma(n - \mu + 1)}{n!} P_n'(x) \right). \end{aligned}$$

We conclude this section with some explicit examples. Given an integer  $k \geq 1$ , we can build the discretization  $D_N^{k+\sigma}$  of  $D^{k+\sigma}$ ,  $0 < \sigma < 1$ , by taking for example, as representation nodes  $x_j$ ,  $j = 1, 2, \dots, N$ , the zeros of the derivative of the Chebyshev polynomial  $T_N$ , with the additional point  $x_N = 1$ , i.e. the nodes defined in (2.7). Moreover, we suppose for the moment that the collocation nodes coincide with the

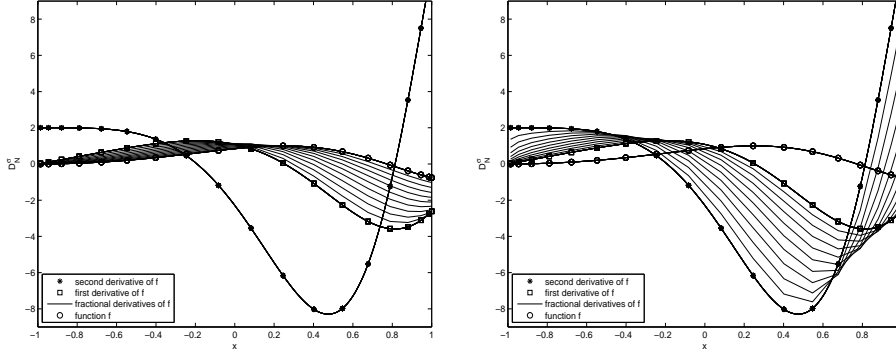


FIG. 1. Fractional derivative approximations  $D_N^\sigma$  of the function  $f(x) = \sin(x+1)^2$  for  $N = 19$ . Here  $\sigma$  varies from 0.1 to 0.9, step 0.1 (left), and from 1.1 to 1.9, step 0.1 (right).

representation nodes; in other words we assume:  $z_i = x_i$ ,  $i = 1, 2, \dots, N$ . In Figure 1, we show the results of some tests. Fractional derivatives of the function  $f(x) = \sin(x+1)^2$  are computed for a given  $N$  and various choices of  $\sigma$ ,  $0 < \sigma < 1$ . The decay of  $f$  near the point  $x_0 = -1$  is quadratic. This allows for a rather good calculation of the derivatives up to the order one. The decay of  $f'$  is just linear and this creates a kind of boundary layer near the point  $x = -1$ . The reason for this behavior can be attributed to the decision of representing  $u_N$  through the basis in (2.2), where the parameter  $\mu = 1 - \sigma$  dictates the decay rate of the discrete fractional derivative at the point  $x = -1$ . In order to handle these specific situations, a less tamed basis should be constructed on purpose, though this is not a subject we shall deal with.

**4. Choice of the collocation nodes.** As we mentioned in the previous section, we are not obliged to choose the set of collocation nodes equal to that used to represent the solution. This observation suggests a series of experiments with different combinations of nodes. Although the choices can be infinite, we will concentrate our attention on some meaningful cases.

First of all, we note that, thanks to (1.5), the derivative of the Jacobi polynomial  $P_N^{(\alpha-1, \beta-1)}$  is proportional to  $P_{N-1}^{(\alpha, \beta)}$ . As suggested in [46], [47], a framework providing very good performances is the one where the representation nodes  $x_j$ ,  $j = 0, 1, \dots, N$ , are the zeros of  $P_{N-1}^{(\alpha, \beta)}$ , with the addition of the points  $x_0 = -1$  and  $x_N = 1$  (see (2.7) concerning the Chebyshev case). Systematically, the collocation nodes are chosen such that  $x_j = z_j$ ,  $j = 1, 2, \dots, N$ . We now examine the possibility of assigning a different set of collocation nodes. We argue as done in [14], [15] and [12].

We start by introducing a function  $\chi_N^{(\alpha, \beta)}$  as follows:

$$(4.1) \quad \chi_N^{(\alpha, \beta)}(x) = (1+x)^\beta (1-x)^\alpha P_{N-1}^{(\alpha, \beta)}(x), \quad x \in [-1, 1],$$

and we consider as nodes  $x_j$ ,  $j = 0, 1, \dots, N$ , the zeros of (4.1), that automatically include the endpoints  $\pm 1$ . Obviously,  $\chi_N^{(\alpha, \beta)}$  vanishes at all points of the grid, thus, the discrete derivative  $D_N^\sigma$  applied to  $\chi_N^{(\alpha, \beta)}$  is identically zero (viewed from the discrete space,  $\chi_N^{(\alpha, \beta)}$  is practically the zero function). We now apply the exact fractional operator  $D^\sigma$  to  $\chi_N^{(\alpha, \beta)}$ . This turns out to be an oscillating function. Successively, we look for collocation nodes such that  $[D^\sigma \chi_N^{(\alpha, \beta)}](z_i) = 0$ ,  $i = 1, 2, \dots, N$ . By this

choice, we must also get:

$$(4.2) \quad [(D^\sigma - D_N^\sigma)\chi_N^{(\alpha,\beta)}](z_i) = 0, \quad i = 1, 2, \dots, N.$$

Such an equation tells us that the operator  $D^\sigma - D_N^\sigma$  not only vanishes on the approximation space (by construction, considering that such a space is the span of the Lagrange type basis (2.2)), but also that the extra element  $\chi_N^{(\alpha,\beta)}$  belongs to the kernel of  $D^\sigma - D_N^\sigma$ . This means that we are able to enlarge the dimension of the approximation space by one unity. As we will check, such an improved consistency property (called *superconsistency*, according to [15]) is the key to obtain optimal numerical results, especially when the degree  $N$  is not large.

In this section, we study both the ultraspherical case, i.e.:  $\alpha = \beta$  (§4.1) and the case  $\alpha = -\beta$  (§4.2) although what we are going to say also holds in a general context.

**4.1. The case  $\alpha = \beta$ .** Let us consider the function:

$$(4.3) \quad \chi_N^{(\alpha,\alpha)}(x) = (1+x)^\alpha(1-x)P_{N-1}^{(\alpha,\alpha)}(x), \quad x \in [-1, 1],$$

and let us assume that the nodes  $x_j$ ,  $j = 0, 1, \dots, N$ , are the zeros of (4.3).

Note that  $T'_N$  is proportional to  $P_{N-1}^{(\alpha,\beta)}$  with  $\alpha = \beta = 1/2$  (see (1.5) and (1.11)). Thus, the Chebyshev case is included in our analysis. In the same way,  $P'_N$  is proportional to  $P_{N-1}^{(\alpha,\beta)}$  with  $\alpha = \beta = 1$  (see (1.5)), so that the Legendre case is also included.

The next step is to develop the polynomial  $(1-x)P_{N-1}^{(\alpha,\alpha)}$  in (4.3) in terms of Jacobi polynomials of the same family. We recall the recurrence relation (1.7) when  $\alpha = \beta$ , so we have:

$$(4.4) \quad \begin{aligned} P_N^{(\alpha,\alpha)}(x) &= a_N x P_{N-1}^{(\alpha,\alpha)}(x) - c_N P_{N-2}^{(\alpha,\alpha)}(x), \\ \text{with} \quad a_N &= \frac{(N+\alpha)(2N+2\alpha-1)}{N(N+2\alpha)}, \quad c_N = \frac{(N+\alpha)(N+\alpha-1)}{N(N+2\alpha)}. \end{aligned}$$

Therefore:

$$(4.5) \quad \chi_N^{(\alpha,\alpha)}(x) = (1+x)^\alpha \left( P_{N-1}^{(\alpha,\alpha)}(x) - \frac{P_N^{(\alpha,\alpha)}(x)}{a_N} - \frac{c_N P_{N-2}^{(\alpha,\alpha)}(x)}{a_N} \right).$$

To avoid cumbersome calculations, we continue the discussion with the case of the Chebyshev Gauss-Lobatto nodes, corresponding to  $\alpha = \beta = 1/2$  (generalizations are however straightforward). The above formula (4.5) takes the form:

$$(4.6) \quad \begin{aligned} \chi_N^{(1/2,1/2)}(x) &= \sqrt{1+x} \left( P_{N-1}^{(1/2,1/2)}(x) - \frac{N+1}{2N+1} P_N^{(1/2,1/2)}(x) \right. \\ &\quad \left. - \frac{2N-1}{4N} P_{N-2}^{(1/2,1/2)}(x) \right). \end{aligned}$$

Let  $\mu = 1 - \sigma$ . We apply the derivative operator  $D^\sigma$  to  $\chi_N^{(1/2,1/2)}$ . By plugging the



combination (4.6) into (1.12) one obtains:

$$\begin{aligned}
 \Psi_N^{(1/2,1/2)}(x) &= (D^\sigma \chi_N^{(1/2,1/2)})(x) = \frac{1}{\Gamma(\mu)} \frac{d}{dx} \int_{-1}^x \frac{\chi_N^{(1/2,1/2)}(s)}{(x-s)^{1-\mu}} ds \\
 &= \frac{d}{dx} \left[ (1+x)^{1/2+\mu} \left( \frac{\Gamma(N+\frac{1}{2})}{\Gamma(N+\frac{1}{2}+\mu)} P_{N-1}^{(1/2-\mu,1/2+\mu)}(x) \right. \right. \\
 (4.7) \quad &\quad \left. \left. - \frac{N+1}{2N+1} \frac{\Gamma(N+\frac{3}{2})}{\Gamma(N+\frac{3}{2}+\mu)} P_N^{(1/2-\mu,1/2+\mu)}(x) \right. \right. \\
 &\quad \left. \left. - \frac{2N-1}{4N} \frac{\Gamma(N-\frac{1}{2})}{\Gamma(N-\frac{1}{2}+\mu)} P_{N-2}^{(1/2-\mu,1/2+\mu)}(x) \right) \right],
 \end{aligned}$$

where we defined  $\Psi_N^{(1/2,1/2)}$  to be the resulting function.

Also easy is the case of the Legendre Gauss-Lobatto nodes, corresponding to  $\alpha = \beta = 1$ . We have:

$$(4.8) \quad \chi_N^{(1,1)}(x) = (1+x) \left[ P_{N-1}^{(1,1)}(x) - \frac{N(N+2)P_N^{(1,1)}(x)}{(N+1)(2N+1)} - \frac{NP_{N-2}^{(1,1)}(x)}{2N+1} \right].$$

Successively, one gets:

$$\begin{aligned}
 \Psi_N^{(1,1)}(x) &= (D^\sigma \chi_N^{(1,1)})(x) = \frac{1}{\Gamma(\mu)} \frac{d}{dx} \int_{-1}^x \frac{\chi_N^{(1,1)}(s)}{(x-s)^{1-\mu}} ds \\
 &= \frac{d}{dx} \left[ (1+x)^{1+\mu} \left( \frac{\Gamma(N+1)}{\Gamma(N+1+\mu)} P_{N-1}^{(1-\mu,1+\mu)}(x) \right. \right. \\
 (4.9) \quad &\quad \left. \left. - \frac{N(N+2)}{(N+1)(2N+1)} \frac{\Gamma(N+2)}{\Gamma(N+2+\mu)} P_N^{(1-\mu,1+\mu)}(x) \right. \right. \\
 &\quad \left. \left. - \frac{N}{2N+1} \frac{\Gamma(N)}{\Gamma(N+\mu)} P_{N-2}^{(1-\mu,1+\mu)}(x) \right) \right].
 \end{aligned}$$

We propose to take the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N$ , to be the zeros of  $\Psi_N^{(\alpha,\beta)}$  for  $\alpha = \beta = 1/2$  or  $\alpha = \beta = 1$ . This actually corresponds to find the zeros of a suitable polynomial of degree  $N$ . Note that  $x = 1$  is not a collocation point.

For some values of  $N$  and  $0 < \mu < 1$ , we show in Figures 2, 3 the plots of the function  $\Psi_N^{(1,1)}$ . The situation is qualitatively the same for other values of the parameters. It turns out that we are rather lucky: there are actually  $N$  zeros of  $\Psi_N^{(1,1)}$  in the interval  $[-1, 1]$  (symbol  $\diamond$  in Figures 2, 3). Therefore, the whole construction seems to have solid foundations, though we do not have a strict proof of this fact. We can point out another singular property. In the pictures we also plot the zeros of the Legendre polynomial  $P_N$  (symbol  $*$  in Figures 2, 3). They are interlaced with our new zeros. This is quite important for numerical reasons, if for instance one wants to seek the collocation nodes through the bisection method.

**4.2. The case  $\alpha = -\beta$ .** Let us consider the case  $\alpha = \mu$ ,  $\beta = -\mu$ , and assume that the nodes  $x_j$ ,  $j = 0, 1, \dots, N$ , are the zeros of  $\frac{d}{dx} P_N^{(\mu, -\mu)}$  plus the endpoints  $\pm 1$ . As in the previous section, we would like to determine the collocation points in order to enlarge the discretization space by including one more function in the kernel of the operator  $D^\sigma - D_N^\sigma$ .

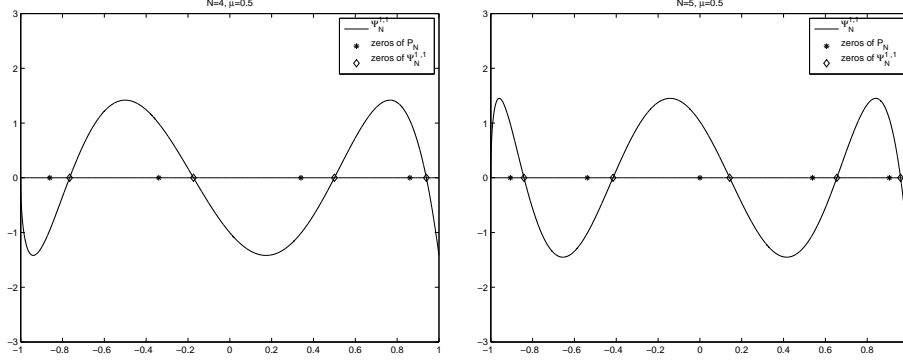


FIG. 2. The function  $\Psi_N^{(1,1)}$  for  $\mu = 0.5$  and  $N = 4$  (left),  $N = 5$  (right).

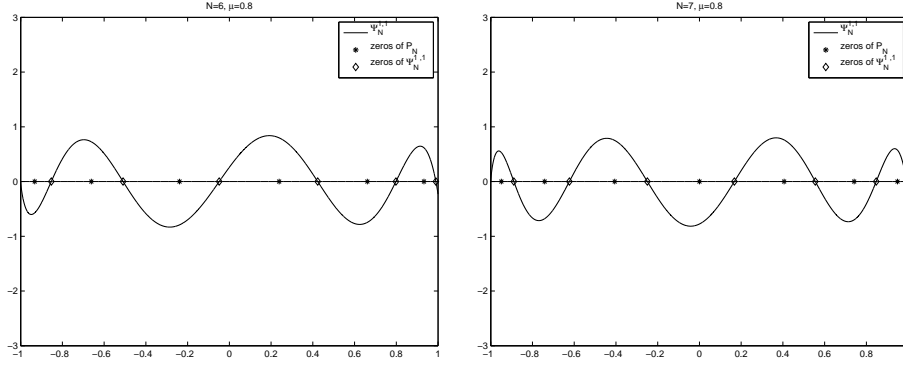


FIG. 3. The function  $\Psi_N^{(1,1)}$  for  $\mu = 0.8$  and  $N = 6$  (left),  $N = 7$  (right).

Similarly to what has been done before, we consider the zeros  $x_j$ ,  $j = 0, 1, \dots, N$ , of the following function:

$$(4.10) \quad \chi_N^{(1+\mu, 1-\mu)}(x) = (1+x)^{1-\mu}(1-x) \frac{d}{dx} P_N^{(\mu, -\mu)}(x).$$

The notation of formula (4.10) is justified from the fact that  $\frac{d}{dx} P_N^{(\mu, -\mu)}$  is proportional to  $P_{N-1}^{(1+\mu, 1-\mu)}$  (see (1.5)), so that:

$$(4.11) \quad \chi_N^{(1+\mu, 1-\mu)}(x) = \frac{N+1}{2} (1+x)^{1-\mu}(1-x) P_{N-1}^{(1+\mu, 1-\mu)}.$$

From (1.7) we have:

$$(4.12) \quad P_N^{(1+\mu, 1-\mu)}(x) = (a_N x + b_N) P_{N-1}^{(1+\mu, 1-\mu)}(x) + c_N P_{N-2}^{(1+\mu, 1-\mu)}(x), \quad \forall N \geq 2,$$

where:

$$(4.13) \quad a_N = \frac{(N+1)(2N+1)}{N(N+2)},$$

$$(4.14) \quad b_N = \frac{\mu(2N+1)}{N^2(N+2)},$$

$$(4.15) \quad c_N = -\frac{(N^2 - \mu^2)(N+1)}{N^2(N+2)}, \quad \forall N \geq 2.$$

As a consequence the following expression for  $\chi_N^{(1+\mu, 1-\mu)}$  holds:

$$(4.16) \quad \begin{aligned} \chi_N^{(1+\mu, 1-\mu)}(x) &= (1+x)^{1-\mu} \frac{N+1}{2} \left[ \left(1 + \frac{b_N}{a_N}\right) P_{N-1}^{(1+\mu, 1-\mu)}(x) \right. \\ &\quad \left. - \frac{1}{a_N} P_N^{(1+\mu, 1-\mu)}(x) + \frac{c_N}{a_N} P_{N-2}^{(1+\mu, 1-\mu)}(x) \right]. \end{aligned}$$

On the other hand, by virtue of (1.5), (1.12) and (2.9), one discovers that:

$$(4.17) \quad \begin{aligned} \int_{-1}^x \frac{(1+s)^{1-\mu} P_n^{(1+\mu, 1-\mu)}(s)}{(x-s)^{1-\mu}} ds &= \frac{\Gamma(\mu)\Gamma(n+2-\mu)}{(n+1)!} (1+x) P_n^{(1,1)}(x) \\ &= \frac{2\Gamma(\mu)\Gamma(n+2-\mu)}{(n+2)!} (1+x) P_{n+1}'(x). \end{aligned}$$

Therefore, by applying  $D^\sigma$  (with  $\mu = 1 - \sigma$ ) to the expression of  $\chi_N^{(1+\mu, 1-\mu)}$  given in (4.16), one finally gets:

$$(4.18) \quad \begin{aligned} \Psi_N^{(1+\mu, 1-\mu)}(x) &= (D^\sigma \chi_N^{(1+\mu, 1-\mu)})(x) \\ &= (N+1) \frac{d}{dx} \left\{ (1+x) \left[ \left(1 + \frac{b_N}{a_N}\right) \frac{\Gamma(N+1-\mu)}{(N+1)!} P_N'(x) \right. \right. \\ &\quad \left. \left. - \frac{1}{a_N} \frac{\Gamma(N+2-\mu)}{(N+2)!} P_{N+1}'(x) + \frac{c_N}{a_N} \frac{\Gamma(N-\mu)}{N!} P_{N-1}'(x) \right] \right\} \\ &= \frac{(N+1)\Gamma(N-\mu)}{N!} \frac{d}{dx} \left\{ (1+x) \frac{d}{dx} \left[ \left(1 + \frac{b_N}{a_N}\right) \frac{N-\mu}{N+1} P_N(x) \right. \right. \\ &\quad \left. \left. - \frac{1}{a_N} \frac{(N+1-\mu)(N-\mu)}{(N+2)(N+1)} P_{N+1}(x) + \frac{c_N}{a_N} P_{N-1}(x) \right] \right\}. \end{aligned}$$

The right-hand side in (4.18) is a polynomial of degree  $N$ . Thus, we suggest to choose the zeros of  $\Psi_N^{(1+\mu, 1-\mu)}$  as collocation nodes.

We can simplify (4.18) by introducing some approximation. For  $N$  large, one has:  $a_N \approx 2$ ,  $c_N \approx -1$ , while  $b_N$  tends to zero. Thus, for  $N$  large we are allowed to write:

$$(4.19) \quad \begin{aligned} &\frac{d}{dx} \left\{ (1+x) \frac{d}{dx} \left[ \left(1 + \frac{b_N}{a_N}\right) \frac{N-\mu}{N+1} P_N(x) \right. \right. \\ &\quad \left. \left. - \frac{1}{a_N} \frac{(N+1-\mu)(N-\mu)}{(N+2)(N+1)} P_{N+1}(x) + \frac{c_N}{a_N} P_{N-1}(x) \right] \right\} \\ &\approx \frac{d}{dx} \left\{ (1+x) \frac{d}{dx} \left[ P_N(x) - \frac{1}{2} P_{N+1}(x) - \frac{1}{2} P_{N-1}(x) \right] \right\}. \end{aligned}$$

On the other hand, by the recurrence relation for Legendre polynomials (see (1.7) for  $\alpha = \beta = 0$ ), we deduce that:

$$(4.20) \quad \frac{1}{2} P_{N+1}(x) + \frac{1}{2} P_{N-1}(x) \approx x P_N(x).$$

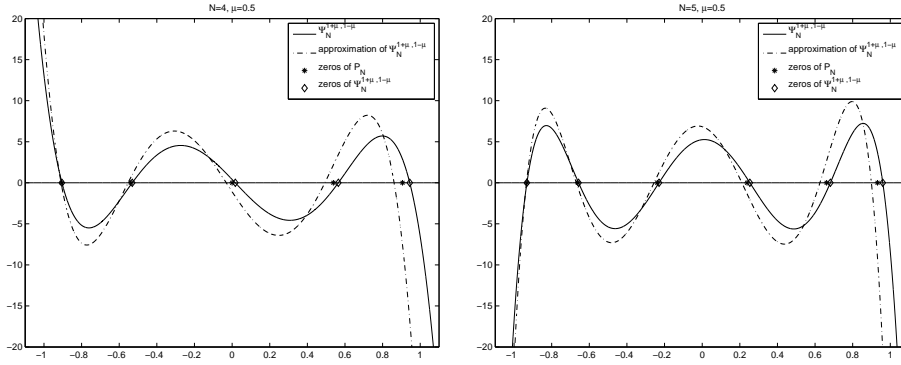


FIG. 4. The function  $\Psi_N^{(1+\mu, 1-\mu)}$ ,  $\mu = 0.5$ , and its approximation for  $N = 4$  (left) and  $N = 5$  (right).

In this way, the right-hand side of (4.19) is approximated by:

$$(4.21) \quad \frac{d}{dx} \left\{ (1+x) \frac{d}{dx} [(1-x)P_N] \right\} = \left( (1-x^2)P_N' \right)' - \left( (1+x)P_N \right)' = -(N^2 + N + 1)P_N - (1+x)P_N',$$

where we used the differential equation characterizing Legendre polynomials (see (1.2) for  $\alpha = \beta = 0$ ). It is worthwhile to observe that these last formulas do not depend on  $\mu$ . Thus, from (4.18) for  $N$  sufficiently large we can write:

$$(4.22) \quad \Psi_N^{(1+\mu, 1-\mu)} \approx -\frac{(N+1)\Gamma(N-\mu)}{N!} [(1+x)P_N' + (N^2 + N + 1)P_N],$$

that could turn out to be useful in order to understand the theoretical properties of the function  $\Psi_N^{(1+\mu, 1-\mu)}$ , such as the location of its zeros. Note that in the above formula the multiplying constant approaches  $(N+1)/N$  for  $\mu \rightarrow 0$  and  $(N+1)/N(N-1)$  for  $\mu \rightarrow 1$ . We expect that the zeros of  $\Psi_N^{(1+\mu, 1-\mu)}$  are not very far from those of the right-hand side in (4.22). As a matter of fact, we compare in Figure 4 the plots of  $\Psi_N^{(1+\mu, 1-\mu)}$  with those of the corresponding approximations, for different values of  $N$  and  $\mu$ . In both cases, there are exactly  $N$  zeros, all belonging to the interval  $] -1, 1[$ . A comparison with the zeros of  $P_N$  is also made (symbol  $*$  in Figure 4). The two sets of points (zeros of  $\Psi_N^{(1+\mu, 1-\mu)}$  and Legendre zeros) are alternate. This has proven to be true for all the values of  $\mu$  and  $N$  that we tested. Having an idea of the distribution of the new collocation points (symbol  $\diamond$  in Figure 4) is important in view of developing methods for their numerical computation. For instance, the implementation of the bisection methods follows naturally. In order to set up the collocation scheme that is discussed in the coming sections, we actually computed the approximate zeros of  $\Psi_N^{(1+\mu, 1-\mu)}$  by the bisection method. For convenience, in Figure 5 we also show the zeros of  $\Psi_N^{(1+\mu, 1-\mu)}$  for  $N = 2$  (symbol  $\diamond$ ) and  $N = 3$  (symbol  $\square$ ) when  $\mu$  varies from 0 to 1 with step 0.1.

**5. Some preliminary numerical results.** Based on what obtained in the previous section, there are many possible ways to approach the fractional differential problem (2.12), through the discrete problem (2.13), depending on the construction

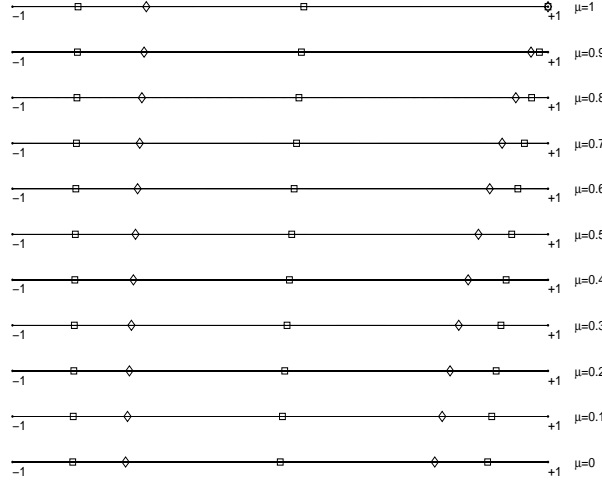


FIG. 5. Zeros of  $\Psi_N^{(1+\mu, 1-\mu)}$  for  $N = 2$  (symbol  $\diamond$ ) and  $N = 3$  (symbol  $\square$ ) for different values of  $\mu$ .

of the discrete fractional operator  $D_N^\sigma$ ,  $0 < \sigma < 1$ . In the examples we are discussing, variants do not only rely on the choice of the initial polynomial basis, but also on the choice of the collocation grid.

In all the cases we are going to examine in this section, given  $0 < \sigma < 1$ , we take  $\mu = 1 - \sigma$  and we represent the function to be differentiated using the grid-points  $x_j$ , taken to be the  $N - 1$  zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  plus the endpoints  $x_N = \pm 1$ . Those correspond to the zeros of the function  $\chi_N^{(1+\mu, 1-\mu)}$  defined in (4.10). One then builds the  $N \times N$  approximation matrices  $D_N^\sigma$  by suitably choosing the collocation nodes  $z_i$ ,  $i = 1, \dots, N$ . For simplicity, we just consider the following possibilities:

- Choice 1* - The representation nodes  $x_j$ ,  $j = 1, 2, \dots, N$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  plus the endpoint  $x_N = 1$  and the collocation nodes coincide with the representation nodes, i.e.,  $z_i = x_i$ ,  $i = 1, 2, \dots, N$ ;
- Choice 2* - The representation nodes  $x_j$ ,  $j = 1, 2, \dots, N$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  plus the endpoint  $x_N = 1$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N$ , are the zeros of the derivative of the Chebyshev polynomial  $T_N$  with the addition of the point  $x_N = 1$ , i.e., the points defined in (2.7);
- Choice 3 (superconsistency)* - The representation nodes  $x_j$ ,  $j = 1, 2, \dots, N$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  plus the endpoint  $x_N = 1$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N$ , are the  $N$  zeros of  $\Psi_N^{(1+\mu, 1-\mu)} = D^\sigma \chi_N^{(1+\mu, 1-\mu)}$ , as defined in (4.18).

The fact that the representation nodes are all the same in these examples will allow us to make appropriate and consistent comparisons.

We start with a problem also examined in [47], where the exact solution is known. The fractional differential problem is the one in (2.12), with right-hand side  $g(x) = [\Gamma(1+\theta)/\Gamma(1+\theta-\sigma)](1+x)^{\theta-\sigma}$ , with  $\theta = 6+9/17$ . In this way, the exact solution turns out to be  $u(x) = (1+x)^\theta$  which is a fractional-order function. We examine the three possibilities itemized above by choosing  $\sigma = 0.5$ . In Table 2 the reader can find the errors in the discrete maximum norm. The best performance is provided by *Choice 3*

TABLE 2

Errors in the discrete maximum norm between the exact solution  $u$  and the approximated solution  $u_N$  of problem (2.12) with  $\sigma = 0.5$  and  $g$  in such a way that the exact solution is  $u(x) = (1+x)^{6+9/17}$ . They are obtained with the same representation nodes, but with different collocation nodes, as a consequence of Choice 1 (Error 1), Choice 2 (Error 2), and Choice 3 (Error 3).

$N$	Error 1	Error 2	Error 3
4	3.6179	8.9055	0.0964
5	0.6886	1.5741	0.0054
6	0.0615	0.1310	9.1182e-06
7	1.4464e-04	2.8950e-04	5.1570e-07
8	1.0394e-05	1.9705e-05	5.9437e-08
9	1.4101e-06	2.5502e-06	1.0054e-08
10	2.6938e-07	4.6759e-07	2.1819e-09
11	6.4529e-08	1.0806e-07	5.6763e-10
12	1.8225e-08	2.9567e-08	1.6976e-10
13	5.8431e-09	9.2168e-09	5.6755e-11
14	2.0734e-09	3.1896e-09	2.0783e-11
15	7.9979e-10	1.2030e-09	8.2083e-12

(Error 3), corresponding to the superconsistent method. Here the errors are hundreds times smaller. Successively, we solve numerically the fractional differential problem (2.12) with  $\sigma = 0.5$  and right-hand side  $g(x) = \sin 2(x+1)^2$ . Note that now the exact solution of  $D^\sigma u = g$  is not known; therefore, we compute an approximation of  $u$  with  $N$  relatively large, to be used in place of  $u$  in our comparisons. It does not matter what set of collocation nodes is utilized in this operation, since, due to spectral convergence, the various approximations are graphically indistinguishable for  $N$  sufficiently large. The solution  $u_N$  of (2.13) is represented through (2.1), with  $H_j$ ,  $j = 1, 2, \dots, N$ , defined in (2.2). The results of these tests are given in Figures 6 and 7 for  $N = 5, 6, 7, 8$ , respectively. Here  $N$  is not large, so that some differences soon emerge, depending on the choice of the collocation sets. The “exact solution” in Figures 6 and 7 has been computed with  $N = 50$  using for both representation and collocation nodes the points defined in (2.7). It is clear from pictures that the approach here proposed provides reasonable approximations, even at such low polynomial degrees, while the more classical methods tend to be less accurate. By enlarging  $N$ , all the three types of approximated solutions converge spectrally. Thus, their plots are almost coincident. We give in Table 3 the corresponding errors. The conclusions are the same of the previous test.

We end this section by showing how to recover the entries of the matrix  $A_N$  in (2.6) in explicit way, when the representation nodes are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}(x_j)$  plus the endpoints  $\pm 1$ . We start by recalling the Gauss-Lobatto integration formula:

$$(5.1) \quad \int_{-1}^1 q(x)(1-x)^\alpha(1+x)^\beta dx = \sum_{m=0}^N q(x_m)w_m,$$

valid for any  $q$  polynomial of degree less or equal to  $2N-1$ . The weights  $w_m$ ,  $m = 0, 1, \dots, N$  are known (see [13], p.52, and [37], p.83). For  $1 \leq k \leq N-1$ , we

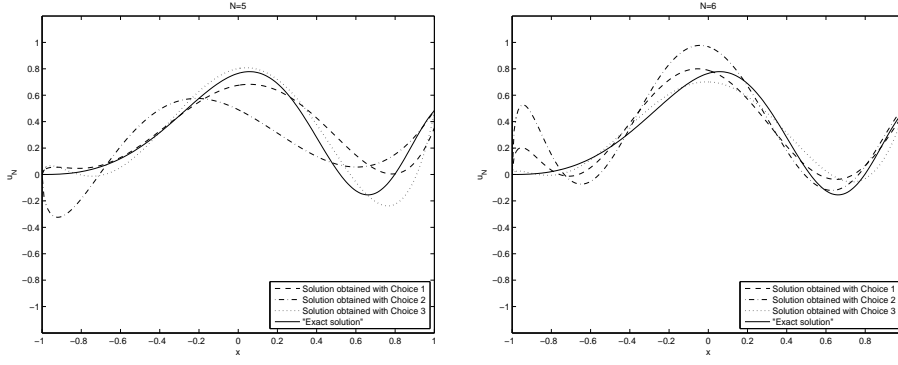


FIG. 6. Approximated solutions for  $N = 5$  and  $N = 6$  of the fractional differential problem (2.12) with  $g(x) = \sin 2(x+1)^2$ ,  $\sigma = 0.5$ , for the three different choices of collocation nodes described in §5.

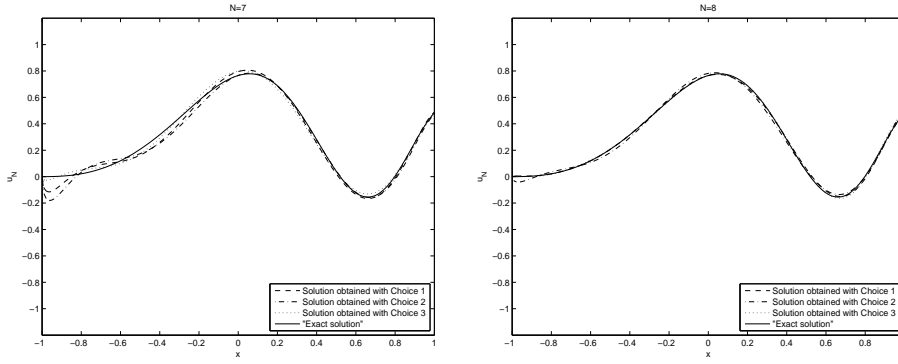


FIG. 7. Approximated solutions for  $N = 7$  and  $N = 8$  of the fractional differential problem (2.12) with  $g(x) = \sin 2(x+1)^2$ ,  $\sigma = 0.5$ , for the three different choices of collocation nodes described in §5.

multiply (2.5) by  $P_k^{(\mu, -\mu)}(x_m)w_m$ ; we then sum up on the index  $m$ , obtaining:

$$\begin{aligned}
 & \sum_{n=1}^N c(j, n) \sum_{m=0}^N \left[ P_n^{(\mu, -\mu)}(x_m) - P_n^{(\mu, -\mu)}(-1) \right] P_k^{(\mu, -\mu)}(x_m) w_m \\
 (5.2) \quad & = \sum_{m=0}^N \delta_{jm} (x_m + 1)^\mu P_k^{(\mu, -\mu)}(x_m) w_m = (x_j + 1)^\mu P_k^{(\mu, -\mu)}(x_j) w_j.
 \end{aligned}$$

Since  $k+n \leq 2N-1$ , we can apply Gaussian integration, and due to the orthogonality of Jacobi polynomials one finally gets:

$$(5.3) \quad c(j, k) \int_{-1}^1 \left[ P_k^{(\mu, -\mu)}(x) \right]^2 (1-x)^\mu (1+x)^{-\mu} dx = (x_j + 1)^\mu P_k^{(\mu, -\mu)}(x_j) w_j,$$

from which one easily gets the coefficients for  $1 \leq j \leq N$  and  $1 \leq k \leq N-1$ . If  $k = N$ , we can still arrive at the expression in (5.2). Successively, we can use the

TABLE 3

Errors in the discrete maximum norm between the “exact solution”  $u$  and the approximated solution  $u_N$  of problem (2.12) with  $\sigma = 0.5$ ,  $g(x) = \sin 2(x+1)^2$ . They are obtained with the same representation nodes, but with different collocation nodes, as a consequence of Choice 1 (Error 1), Choice 2 (Error 2), and Choice 3 (Error 3).

$N$	Error 1	Error 2	Error 3
4	0.4057	0.6852	0.0824
5	0.2053	0.3807	0.0363
6	0.1348	0.4069	0.0084
7	0.0764	0.1365	0.0039
8	0.0140	0.0316	0.0015
9	0.0143	0.0417	3.7184e-04
10	0.00653	0.0128	1.1357e-04
11	5.4582e-04	0.0012	4.7035e-05
12	7.0567e-04	0.0021	1.1296e-05
13	3.1975e-04	6.8793e-04	1.9664e-06
14	3.7780e-05	2.4258e-05	9.9621e-07
15	1.9172e-05	6.1681e-05	2.5710e-07

orthogonality when the index  $n$  is between 1 and  $N-1$ . In the end, we get:

$$(5.4) \quad c(j, N) \sum_{m=0}^N \left[ P_N^{(\mu, -\mu)}(x_m) \right]^2 w_m = (x_j + 1)^\mu P_N^{(\mu, -\mu)}(x_j) w_j,$$

from which one recovers  $c(j, N)$ , for  $1 \leq j \leq N$ .

**6. Application to a boundary-value problem.** In this last section, we would like to approximate the solution  $u$  of the following differential fractional equation with homogeneous Dirichlet boundary constraints:

$$(6.1) \quad -\frac{d^2 u}{dx^2} + K D^\sigma u = g, \quad \text{with } u(\pm 1) = 0,$$

where  $0 < \sigma < 1$ , and  $K$  is a given constant. Throughout this section we take  $\mu = 1 - \sigma$ . In finite dimension, problem (6.2) reads as follows:

$$(6.2) \quad -D_N^2 u_N + K D_N^\sigma u_N = g_N, \quad \text{with } u_N(\pm 1) = 0,$$

and this equation must hold at some collocation points.

The solution  $u_N$  of (6.2) is represented as in (2.1) with  $H_j$ ,  $j = 1, 2, \dots, N$ , defined in (2.2). Since we want to impose boundary conditions, the sum in (2.1) goes from  $j = 1$  up to  $j = N-1$ . Once the representation points  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are chosen, the approximating matrix is recovered by applying the discrete operator  $-D_N^2 + K D_N^\sigma$  to  $H_j$  and evaluating at the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N-1$ .

From the results of the previous sections, several possibilities may be taken into account both for the representation grid and the collocation grid. In order to get *superconsistent* type approximations, the following possibilities are considered.

1) The representation nodes  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are the zeros of  $T'_N$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N-1$ , are chosen such that:

$$(6.3) \quad -\chi_N''(z_i) + K \Psi_N(z_i) = 0,$$

where  $\chi_N = \chi_N^{(1/2, 1/2)}$  is defined in (4.6) and  $\Psi_N = \Psi_N^{(1/2, 1/2)}$  is given in (4.7). The above equation actually admits  $N-1$  roots in the interval  $] -1, 1[$ . This leads us to a squared matrix of dimension  $(N-1) \times (N-1)$ .



2) The representation nodes  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are the zeros of  $P'_N$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N-1$ , are the solution of equation (6.3) with  $\chi_N = \chi_N^{(1,1)}$  defined in (4.8) and  $\Psi_N = \Psi_N^{(1,1)}$  obtained from (4.9).

3) The representation nodes  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N-1$ , are the solution of equation (6.3) with  $\chi_N = \chi_N^{(1+\mu, 1-\mu)}$  defined in (4.10) and  $\Psi_N = \Psi_N^{(1+\mu, 1-\mu)}$  computed in (4.18).

We now concentrate our attention on point 3) by carrying out some tests, aimed to compare (as we did in §5) the technique here proposed with the more standard ones. We solve numerically the fractional differential problem (6.1) in the following circumstances:

*Choice 4* - The representation points  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  and the collocation nodes coincide with the representation nodes, i.e.,  $z_i = x_i$ ,  $i = 1, 2, \dots, N-1$ ;

*Choice 5* - The representation points  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N-1$ , are the zeros of the derivative of the Chebyshev polynomial  $T_N$  plus the point  $x_N = 1$ , i.e. the points defined in (2.7);

*Choice 6* (*Superconsistency*, see option 3) above) - The representation points  $x_j$ ,  $j = 1, 2, \dots, N-1$ , are the zeros of  $\frac{d}{dx}P_N^{(\mu, -\mu)}$  and the collocation nodes  $z_i$ ,  $i = 1, 2, \dots, N-1$ , are the  $N-1$  zeros of (6.3) where  $\chi_N = \chi_N^{(1+\mu, 1-\mu)}$  is defined in (4.10) and  $\Psi_N = \Psi_N^{(1+\mu, 1-\mu)}$  is computed in (4.18).

Note that in order to approach the boundary-value problem (6.1) we also need to evaluate the second derivative of  $\chi_N = \chi_N^{(1+\mu, 1-\mu)}$  defined in (4.10). To this scope, let us note that from (1.2) with  $\alpha = \mu$  and  $\beta = -\mu$ , one has:

$$(6.4) \quad \frac{d}{dx} \left[ (1-x^2) \frac{d}{dx} P_N^{(\mu, -\mu)} \right] = 2\mu \frac{d}{dx} P_N^{(\mu, -\mu)} - N(N+1) P_N^{(\mu, -\mu)},$$

and consequently:

$$\begin{aligned} \frac{d^2}{dx^2} \left[ (1+x)^{-\mu} (1-x^2) \frac{d}{dx} P_N^{(\mu, -\mu)} \right] &= \mu(\mu+1)(1+x)^{-\mu-2} (1-x^2) \frac{d}{dx} P_N^{(\mu, -\mu)} \\ &\quad - 2\mu(1+x)^{-\mu-1} \frac{d}{dx} \left[ (1-x^2) \frac{d}{dx} P_N^{(\mu, -\mu)} \right] + (1+x)^{-\mu} \frac{d^2}{dx^2} \left[ (1-x^2) \frac{d}{dx} P_N^{(\mu, -\mu)} \right] \\ (6.5) &= (1+x)^{-\mu-2} [\mu(\mu+1)(1-x^2) - 4\mu^2(1+x) - N(N+1)(1+x)^2] \frac{d}{dx} P_N^{(\mu, -\mu)} \\ &\quad + 2\mu N(N+1)(1+x)^{-\mu-1} P_N^{(\mu, -\mu)} + 2\mu(1+x)^{-\mu} \frac{d^2}{dx^2} P_N^{(\mu, -\mu)}. \end{aligned}$$

In the first numerical test, we discretize the fractional differential problem (6.1) with  $\sigma = 0.5$ ,  $K = 10$  and  $g(x) = 1$ . This is a kind of advection-diffusion problem, with a boundary layer developing on the right-hand side. The behavior in the middle is regulated by the fractional derivative operator. We then compare the results obtained by implementing different sets of collocation nodes as specified above. As done in §5, since the exact solution is not available, we substitute it with an approximation obtained with  $N$  sufficiently large. Figure 8 shows the results of this test for  $N = 4, 5$ , respectively. The superiority of our method is evident, as is also illustrated by the results of Table 4 where the errors in the discrete maximum norm, relative to the cases examined, are shown.

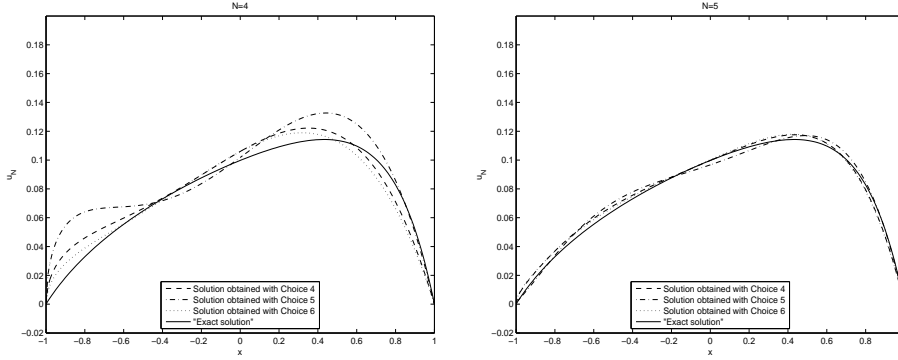


FIG. 8. Approximated solutions for  $N = 4$  and  $N = 5$  of the fractional differential problem (6.1) with  $\sigma = 0.5$ ,  $K = 10$ ,  $g(x) = 1$ , for the three different choices of collocation nodes introduced in §6.

TABLE 4

Errors in the discrete maximum norm between the “exact solution”  $u$  and the approximated solution  $u_N$  of problem (6.1) with  $\sigma = 0.5$ ,  $K = 10$  and  $g(x) = 1$ . They are obtained with the same representation nodes, but with different collocation nodes, as a consequence of Choice 4 (Error 4), Choice 5 (Error 5), and Choice 6 (Error 6).

$N$	Error 4	Error 5	Error 6
4	0.0111	0.0276	0.0045
5	0.0039	0.0049	0.0040
6	0.0049	0.0073	0.0030
7	0.0032	0.0033	0.0024
8	0.0028	0.0033	0.0019
9	0.0022	0.0025	0.0016
10	0.0018	0.0020	0.0013
11	0.0015	0.0017	0.0011
12	0.0013	0.0014	9.2276e-04
13	0.0011	0.0012	7.8751e-04
14	9.5253e-04	0.0010	6.7687e-04
15	8.2687e-04	8.9419e-04	5.8520e-04

In the second test we have  $\sigma = 0.8$ ,  $K = -10$  and  $g(x) = 1$ . Now, the transport is from left to right. Figures 9 and 10 show the results for  $N = 4, 5, 6, 7$ . Again, the best performance is obtained through the superconsistent method. The “exact solutions” shown in Figures 8, 9 and 10 have been actually replaced by approximated ones, obtained for  $N = 50$  by using for both representation and collocation nodes the points defined in (2.7).

Note that, for some critical values of the parameters  $\sigma$ ,  $K$ ,  $N$ , the superconsistent method may blow up, mainly because the procedure for computing the collocation nodes fails. In truth, these are situations where the problem is particularly stiff ( $N$  small,  $|K|$  large), a setting that may constitute a difficulty for any numerical technique. If one stays within reasonable limits, our approach looks reliable and effective.

In conclusion, it may be worthwhile to spend some efforts in computing the “right” set of collocation nodes (that depend on the representation nodes and the differential operator to be approximated), since, with no additional cost, the procedure turns out to be highly accurate and competitive, even if compared with more standard high-order pseudospectral techniques.

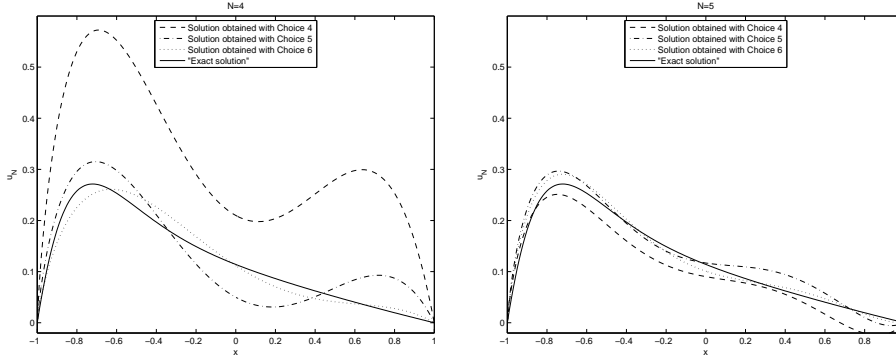


FIG. 9. Approximated solutions for  $N = 4$  and  $N = 5$  of the fractional differential problem (6.1) with  $\sigma = 0.8$ ,  $K = -10$ ,  $g(x) = 1$ , for the three different choices of collocation nodes introduced in §6.

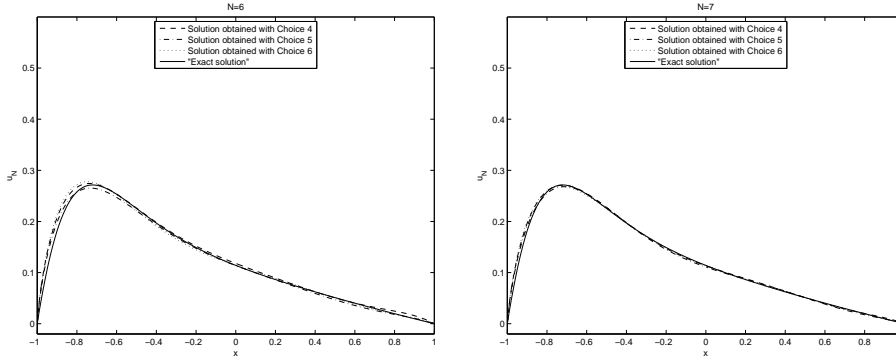


FIG. 10. Approximated solutions for  $N = 6$  and  $N = 7$  of the fractional differential problem (6.1) with  $\sigma = 0.8$ ,  $K = -10$ ,  $g(x) = 1$ , for the three different choices of collocation nodes introduced in §6.

## REFERENCES

- [1] R. ASKEY, AND J. FITCH, *Integral representations for Jacobi polynomials and some applications*, J. Math. Anal. Appl., 26 (1969), pp. 411-437.
- [2] E. BARKAI, R. METZLER, AND J. KLAFTER, *From continuous time random walks to the fractional Fokker-Planck equation*, Phys. Rev. E, 61 (2000), pp. 132-138.
- [3] D. A. BENSON, S. W. WHEATCRAFT, AND M. M. MEERSCHAERT, *Application of a fractional advection-dispersion equation*, Water Resour. Res., 36 (2000), pp. 1403-1412.
- [4] A. S. CHAVES, *A fractional diffusion equation to describe Lévy flights*, Phys. Lett. A, 239 (1998), pp. 13-16.
- [5] W. H. DENG, *Finite element method for the space and time fractional Fokker-Planck equation*, SIAM J. Numer. Anal., 47 (2008), pp. 204-226.
- [6] W. H. DENG, AND C. LI, *Finite difference methods and their physical constraints for the fractional Klein-Kramers equation*, Numer. Methods Partial Differential Equations, 27 (2011), pp. 1561-1583.
- [7] K. DIETHELM, AND N. J. FORD, *Analysis of fractional differential equations*, J. Math. Anal. Appl., 265 (2002), pp. 229-248.
- [8] K. DIETHELM, N. J. FORD, AND A. D. FREED, *Detailed error analysis for a fractional Adams method*, Numer. Algorithms, 36 (2004), pp. 31-52.
- [9] V. J. ERVIN, AND J. P. ROOP, *Variational formulation for the stationary fractional advection dispersion equation*, Numer. Methods Partial Differential Equations, 22 (2006), pp. 558-

- 576.
- [10] V. J. ERVIN, AND J. P. ROOP, *Variational formulation for the fractional advection dispersion equations on bounded domains in  $R^d$* , Numer. Methods Partial Differential Equations, 23 (2007), pp. 256-281.
- [11] V. J. ERVIN, N. HEUER, AND J. P. ROOP, *Numerical approximation of a time dependent, nonlinear, space-fractional diffusion equation*, SIAM J. Numer. Anal., 45 (2007), pp. 572-591.
- [12] L. FATONE, D. FUNARO, AND V. SCANNAVINI, *Finite-differences preconditioners for superconsistent pseudospectral approximations*, ESAIM Math. Model. Numer. Anal., 41-6 (2007), pp. 1021-1039.
- [13] D. FUNARO, *Polynomial Approximation of Differential Equations*, Lecture Notes in Physics Monographs, Volume 8, Springer-Verlag, New York, 1992.
- [14] D. FUNARO, *Spectral Elements for Transport-Dominated Equations*, Lecture Notes In Computational Science and Engineering, Volume 1, Springer-Verlag, New York, 1997.
- [15] D. FUNARO, *Superconsistent discretizations*, J. Sci. Comput., 17 (2002), pp. 67-79.
- [16] D. FUNARO, *Superconsistent discretizations of integral type equations*, Appl. Numer. Math., 48 (2004), pp. 1-11.
- [17] R. GORENFLO, F. MAINARDI, D. MORETTI, AND P. PARADISI, *Time fractional diffusion: a discrete random walk approach*, Nonlinear Dynam., 29 (2002), pp. 129-143.
- [18] B. HENRY, AND S. WEARNE, *Fractional reaction-diffusion*, Phys. A, 276 (2000), pp. 448-455.
- [19] J. S. HESTHAVEN, S. GOTTLIEB, AND D. GOTTLIEB, *Spectral Methods for Time-Dependent Problems*, Cambridge University Press, 2007.
- [20] M. M. KHADER, *On the numerical solutions for the fractional diffusion equation*, Commun. Nonlinear Sci. Numer. Simul., 16 (2011), pp. 2535-2542.
- [21] M. M. KHADER, AND A. S. HENDY, *The approximate and exact solutions of the fractional-order delay differential equations using Legendre pseudospectral method*, Inter. J. Pure Appl. Math., 74 (2012), pp. 287-297.
- [22] T. LANGLANDS, AND B. HENRY, *The accuracy and stability of an implicit solution method for the fractional diffusion equation*, J. Comput. Phys., 205 (2005), pp. 719-736.
- [23] X. LI, AND C. XU, *A space-time spectral method for the time fractional diffusion equation*, SIAM J. Numer. Anal., 47 (2009), pp. 2108-2131.
- [24] X. LI, AND C. XU, *Existence and uniqueness of the weak solution of the space-time fractional diffusion equation and a spectral method approximation*, Commun. Comput. Phys., 8 (2010), pp. 1016-1051.
- [25] Y. LIN, AND C. XU, *Finite difference/spectral approximations for the time-fractional diffusion equation*, J. Comput. Phys., 225 (2007), pp. 1533-1552.
- [26] F. LIU, M. M. MEERSCHAERT, R. J. MCGOUGH, P. ZHUANG, AND Q. LIU, *Numerical methods for solving the multi-term time-fractional wave-diffusion equation*, Fract. Calc. Appl. Anal., 16 (2013), pp. 9-25.
- [27] Q. LIU, F. LIU, I. TURNER, AND V. ANH, *Approximation of the Levy-Feller advection-dispersion process by random walk and finite difference method*, J. Comput. Phys., 222 (2007), pp. 57-70.
- [28] C. LUBICH, *Discretized fractional calculus*, SIAM J. Math. Anal., 17 (1986), pp. 704-719.
- [29] R. L. MAGIN, *Fractional Calculus in Bioengineering*, Begell House, Redding CT, 2006.
- [30] F. MAINARDI, *Fractional Calculus and Waves in Linear Viscoelasticity: An Introduction to Mathematical Models*, Imperial College Press, London, 2010.
- [31] M. M. MEERSCHAERT, AND C. TADJERAN, *Finite difference approximations for fractional advection-dispersion flow equations*, J. Comput. Appl. Math., 172 (2004), pp. 65-77.
- [32] M. M. MEERSCHAERT, AND C. TADJERAN, *Finite difference approximations for two-sided space-fractional partial differential equations*, Appl. Numer. Math., 56 (2006), pp. 80-90.
- [33] R. METZLER, AND J. KLAFTER, *The random walks guide to anomalous diffusion: a fractional dynamics approach*, Phys. Rep., 339 (2000), pp. 1-77.
- [34] R. METZLER, AND J. KLAFTER, *The restaurant at the end of the random walk: recent developments in the description of anomalous transport by fractional dynamics*, J. Phys. A: Math. Gen., 37 (2004), pp. R161-R208.
- [35] A. PABLO, F. QUIRÓS, A. RODRIGUEZ, AND J. L. VÁZQUEZ, *A fractional porous medium equation*, Adv. Math., 226 (2011), pp. 1378-1409.
- [36] I. PODLUBNY, *Fractional Differential Equations*, Academic Press, San Diego CA, 1999.
- [37] J. SHEN, T. TANG, AND L. -L. WANG, *Spectral Methods, Algorithms, Analysis and Applications*, Springer Series in Computational Mathematics, 41, Springer, Heidelberg, 2011.
- [38] N. SUGIMOTO, *Burgers equation with a fractional derivative: hereditary effects on nonlinear acoustic waves*, J. Fluid Mech., 225 (1991), pp. 631-653.

- [39] N. SUGIMOTO, AND T. KAKUTANI, *Generalized Burgers equation for nonlinear viscoelastic waves*, Wave Motion, 7 (1985), pp. 447-458.
- [40] Z. SUN, AND X. WU, *A fully discrete difference scheme for a diffusion-wave system*, Appl. Numer. Math., 56 (2006), pp. 193-209.
- [41] G. SZEGÖ, *Orthogonal Polynomials*, American Mathematical Society, New York, 1939.
- [42] W. Y. TIAN, W. DENG, AND Y. WU, *Polynomial spectral collocation method for space fractional advection-diffusion equation*, Numer. Methods Partial Differential Equations , 30-2 (2014), pp. 514-535.
- [43] L. -L. WANG, X. ZHAO, AND Z. ZHANG, *Superconvergence of Jacobi-Gauss-type spectral interpolation*, J. Sci. Comput., 59 (2014), pp. 667-687.
- [44] G. M. ZASLAVSKY, *Chaos, fractional kinetic, and anomalous transport*, Phys. Rep., 371 (2002), pp. 461-580.
- [45] M. ZAYERNOURI, AND G. E. KARNIADAKIS, *Fractional Sturm-Liouville eigen-problems: theory and numerical approximations*, J. Comput. Phys., 47 (2013), pp. 2108-2131.
- [46] M. ZAYERNOURI, AND G. E. KARNIADAKIS, *Exponentially accurate spectral and spectral element methods for fractional ODEs*, J. Comput. Phys., 257 (2014), pp. 460-480.
- [47] M. ZAYERNOURI, AND G. E. KARNIADAKIS, *Fractional spectral collocation method*, SIAM J. Sci. Comput., 36 (2014), pp. A40-A62.
- [48] H. ZHANG, F. LIU, AND V. ANH, *Garlerkin finite element approximations of symmetric space-fractional partial differential equations*, Appl. Math. Comput., 217 (2010), pp. 2534-2545.
- [49] Z. ZHANG, *Superconvergence points of polynomial spectral interpolation*, SIAM J. Numer. Anal., 50 (2012), pp. 2966-2985.